# Part II: Coordinate Descent Algorithm

## 2.1. Introduction

In this part, we aim to apply the 'one-at-a-time' coordinate descent type of algorithm to solve the penalized regression problems – the lasso problem and elastic net – and to analyse its performance. We first develop our coordinate descent algorithms to solve the lasso penalty and the elastic net penalty, after which we simulate the data. We then obtain the tuning parameters for our models by performing k-fold cross validation using the mean-squared error (MSE) values. Finally, we consider the following scenarios:

- Case I: n > p
- Case II: p > n

when pairwise correlations between the group of variables are very high, and also when $X_i$'s are uncorrelated.

## 2.2. Coordinate Descent Algorithm for Lasso

To solve the Lasso problem, we employ the coordinate descent approach as demonstrated below. The vector of coefficients β is returned by our function lasso_coordinate_descent(X, y, lambda, max_iter = 500, tol = 1e-6) when the parameters are passed in as arguments.

1. We start by initializing βj and $\beta j^{old} = 0$, j = 1,..., p.

2. Until the approach converges for j = 1,..., p, we continue to execute the below mentioned steps:
   a. Let $\beta_j^{old} = \beta_j$. We compute the partial residual by taking:

$$r_{ij} = y_i - \sum_{k \neq j} x_{ik}\beta_k$$

   b. For the j-th predictor, we compute the simple least square coefficients of residuals ($r_{ij}$):

$$\beta_j^* = \frac{1}{n}\sum_{i=1}^{n} x_{ij} r_{ij}$$

   c. Using the soft thresholding approach, we can calculate $\beta_j$ as follows:

$$\beta_j = \text{sign}(\beta_j^*) \max((|\beta_j^*| - \lambda), 0)$$

3. The *max(abs(beta – beta_old)) < tol* checks whether the maximum absolute difference between the elements of the current *beta* estimate and the previous *beta_old* estimate is smaller than a given tolerance, *tol* i.e., $10^{-6}$.

   When this condition becomes TRUE, it means that the change in coefficients between successive iterations has become sufficiently small, indicating convergence or reaching a point where the change in coefficients is negligible according to the tolerance level specified by *tol*. At this point, the algorithm is likely to stop further iterations to avoid unnecessary computation and to consider the current *beta* estimate as the solution.

## 2.3. Coordinate Descent Algorithm for Elastic Net

The coordinate descent algorithm for the elastic net problem is very similar to the algorithm used to solve the lasso, except for a modification to the soft thresholding in the algorithm as follows:

$$\beta_j = \text{sign}(\beta_j^*) \max((|\beta_j^*| - \lambda_1), 0) (1+2\lambda_2)^{-1}$$

## 2.4. Data Simulation Settings

We simulate the data via the model:

$$y = X\boldsymbol{\beta} + \boldsymbol{\sigma\varepsilon},$$

$$\boldsymbol{\varepsilon} \sim N(0, I_n)$$

We first set the parameters to the default values as follows:

- $n = 240$
- $\boldsymbol{\beta} = (3, 1.5, 0, 0, 2, 0, 0, 0)^T$
- $\boldsymbol{\sigma} = 3$
- The pairwise correlations between $X_i$, $X_j$ is determined as: $\text{corr}(X_i, X_j) = 0.5^{|i-j|}$
- r (number of simulations of the entire process) = 50

The code conducts 50 simulations and initiates by setting simulation parameters, including n, p, and the true coefficients for the linear model.

Subsequently, a data frame named 'final' is created to store the results of 50 simulations, with columns representing lambda values (of lasso), lambda_1 and lambda_2 values (of elastic net), the count of nonzero coefficients for both lasso and elastic net (beta_ct_lasso and beta_ct_en), and mean-squared errors for each problem (mse_lasso and mse_en).

## 2.5. Selection of the Regularization Parameters

After simulating the datasets for X and Y, we select optimal tuning parameters, namely $\lambda$ in the lasso algorithm and $\lambda_1$, $\lambda_2$ in the elastic net algorithm.

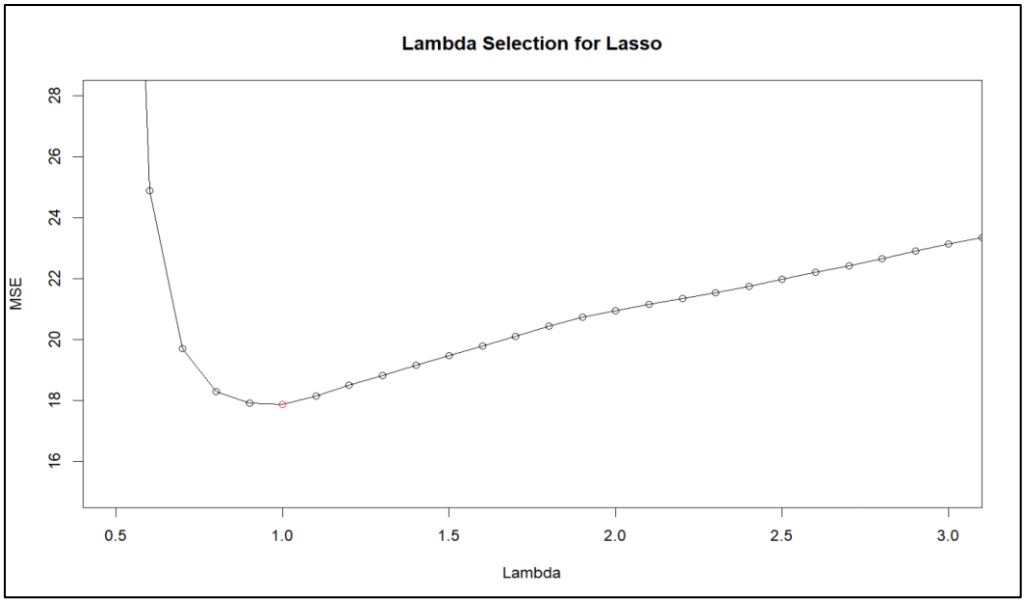
The approach involves a trial-and-error process, in which different values of $\lambda$ are tested on the training dataset. This entails fitting a range of $\lambda$ into the lasso and elastic net functions and evaluating the returned $\beta$ coefficients on the validation data. To validate the data, we use the k-folds cross validation method, via which we divided the data into 12 folds (so as to have 20 data points in each fold for our case of n = 240).

To create the folds, we randomly assigned each row of the simulated data a number between 1 to 12 such that each number occurred 20 times. Running a *for* loop, we then curated the training data by picking those rows which had the key values in the *for* loop. For example, when i = 2, all the rows having fold values as 2 are selected as the training data.

The optimal parameter $\lambda$ is chosen based on the smallest error (MSE) observed on the validation data. To select the optimal tuning parameter we ran the algorithm using trial values in the range of 0 to 5 with an increment of 0.1. Subsequently, the model is re-estimated on the training data using the optimal tuning parameters, and final results are obtained by evaluating it on the test data.

To illustrate the selection of the optimal lambda, we have the following plot showing the lambda selection for the lasso problem by plotting lambda values against the MSE, when solved using the coordinate descent algorithm (for n = 240 and p = 8).

The optimal value of lambda has been highlighted as a red point in the plot.




## 2.6. Main Simulation Results

We get the following results for different cases.

### 2.6.1. In the case: n > p

Within a loop iterating over 50 simulations, datasets are generated with uncorrelated predictors, and cross-validation is employed to estimate optimal regularization parameters. The data is then split into training and test sets, and lasso and elastic net models are fitted using coordinate descent algorithms.

The code calculates relevant metrics, including the count of nonzero coefficients and mean-squared errors for both methods, storing the results in the 'final' data frame, providing a comprehensive basis for comparing the predictive accuracy of the two regularization methods across multiple simulated scenarios. The 'final' data frame is as follows:

| | lambda | lambda_1 | lambda_2 | beta_ct_lasso | beta_ct_en | mse_lasso | mse_en |
|---|---|---|---|---|---|---|---|
| **1** | 1.6 | 1.0 | 0 | 1 | 3 | 22.68513 | 17.45866 |
| **2** | 1.6 | 1.0 | 0 | 2 | 3 | 14.37467 | 10.38992 |
| **3** | 1.8 | 1.5 | 0 | 1 | 2 | 18.67773 | 16.45162 |
| **4** | 2.3 | 1.4 | 0 | 1 | 1 | 18.81744 | 16.02111 |
| **5** | 3.0 | 1.8 | 0 | 1 | 1 | 23.16377 | 18.30002 |
| **6** | 1.5 | 1.3 | 0 | 1 | 2 | 15.40055 | 14.81586 |
| **7** | 2.0 | 1.3 | 0 | 2 | 3 | 15.01681 | 12.05139 |
| **8** | 5.0 | 1.3 | 0 | 0 | 4 | 25.84143 | 12.21610 |
| **9** | 2.5 | 1.3 | 0 | 1 | 2 | 17.63263 | 13.02503 |
| **10** | 3.6 | 1.3 | 0 | 0 | 3 | 29.07759 | 16.76900 |

In this data frame, beta_ct_lasso and beta_ct_rn refer to the number of non-zero coefficients under lasso and elastic net respectively. The columns mse_lasso and mse_en refer to the mean square errors (MSEs) obtained under lasso and elastic net respectively.

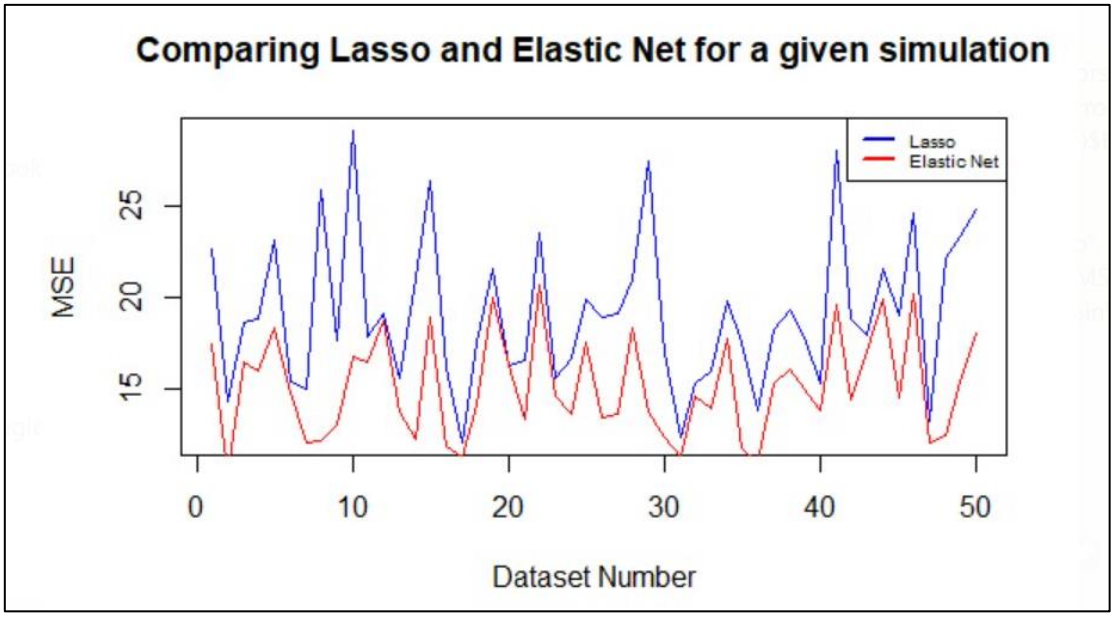
As expected, it is apparent simply from the resulting data frame that elastic net not only dominates lasso in terms of predictive accuracy (because it clearly has less MSE than the lasso in every simulation) but also does a good job in variable selection (it has equal or greater non-zero coefficients in every simulation). To further prove this, we compute:

- the mean and standard error of mean-squared errors mse_lasso and mse_en
- number of estimated non-zero coefficients

In the case n = 240 and p = 8, we have across 50 simulations:

- The mean of MSE for lasso is 19.19177, which is greater than the mean of MSE for elastic net which is 15.15362. The standard error of MSE for lasso = 4.094770, which is greater than standard error of MSE for elastic net which is 2.767536. Thus, we can conclude that **the elastic net has a better predictive performance**.
- On average the number of estimated non-zero coefficients selected by lasso is 1.36, which is less than that for elastic net which is 2.26 on average. Hence, we can conclude that **the elastic net regularization does better than the lasso at variable selection**.

The figure below demonstrates how elastic net clearly dominates over lasso due to lesser mean-squared error values.




To also know whether these results vary with a change in the number of observations, we repeated the simulations to get further results which are explored in section 2.7.

### 2.6.2. In the case: n < p

When p is significantly larger than n, the elastic net penalty demonstrates greater accuracy compared to lasso, especially when data availability is scarce/limited for estimating numerous coefficients. Conversely, when the number of variables is small, the elastic net regularization tends to converge towards lasso regularization.

## 2.7. Additional Simulation Settings – Uncorrelated and Correlated Variables

We had set our default case as n = 240, p = 8 and sd = 3 (as demonstrated before). Then, we attempted to run the code for different values of each of these one at a time while keeping the other parameters constant.

We obtained the following data frame of results, where in the *corr* column 0 represents the case of uncorrelated variables while 1 represents the case of correlated variables.

| n | p | r | sd | b_ct_l | b_ct_en | mse_l_mn | mse_en_mn | mse_l_se | mse_en_se | corr |
|---|---|---|---|---|---|---|---|---|---|---|
| 240 | 8 | 50 | 3 | 1.36 | 2.26 | 19.19177 | 1.515362e+01 | 4.094770 | 2.767536e+00 | 0 |
| 300 | 8 | 50 | 3 | 0.98 | 1.52 | 12.98497 | 1.099103e+01 | 9.584762 | 8.133318e+00 | 0 |
| 240 | 8 | 50 | 3 | 1.34 | 3.00 | 22.35557 | 1.411652e+01 | 5.934406 | 2.872526e+00 | 1 |
| 300 | 8 | 50 | 3 | 1.64 | 2.92 | 20.49657 | 1.468127e+01 | 5.071451 | 3.575724e+00 | 1 |
| 360 | 8 | 50 | 3 | 1.54 | 2.98 | 21.07916 | 1.425221e+01 | 6.075766 | 3.161995e+00 | 1 |
| 360 | 8 | 50 | 3 | 1.40 | 2.40 | 19.27010 | 1.539559e+01 | 4.786475 | 3.609423e+00 | 0 |
| 240 | 10 | 50 | 3 | 1.90 | 4.48 | 22.73571 | 1.518627e+01 | 5.037378 | 3.748489e+00 | 0 |
| 240 | 10 | 50 | 3 | 2.10 | 5.18 | 26.92111 | 1.301449e+135 | 7.550438 | 9.182887e+135 | 1 |
| 240 | 6 | 50 | 3 | 1.58 | 3.26 | 20.85109 | 1.123075e+87 | 7.099948 | 7.941340e+87 | 1 |
| 240 | 6 | 50 | 3 | 1.78 | 2.80 | 17.80067 | 1.362982e+01 | 4.897838 | 3.589545e+00 | 0 |
| 240 | 8 | 50 | 4 | 0.62 | 1.92 | 28.85445 | 2.406992e+01 | 3.619478 | 3.455140e+00 | 0 |
| 240 | 8 | 50 | 4 | 1.14 | 2.68 | 31.34749 | 2.268646e+01 | 5.646062 | 3.977857e+00 | 1 |
| 240 | 8 | 50 | 5 | 0.78 | 2.36 | 42.39783 | 3.347799e+01 | 5.493519 | 5.024903e+00 | 1 |
| 240 | 8 | 50 | 5 | 0.30 | 1.34 | 39.19748 | 3.517070e+01 | 3.194688 | 3.875441e+00 | 0 |
| 240 | 8 | 50 | 6 | 0.26 | 0.78 | 50.74887 | 4.815875e+01 | 3.838985 | 3.985807e+00 | 0 |
| 240 | 8 | 50 | 6 | 0.56 | 2.02 | 54.93928 | 4.646951e+01 | 5.171071 | 5.398852e+00 | 1 |

### 2.7.1. Changing the values of n

There's a sensitivity in lasso and elastic net performance to variations in the number of observations (n). Both approaches often gain from a larger dataset as sample sizes rise, which could result in more precise coefficient estimations. When the number of predictors (p) is minimal compared to the number of observations, lasso can potentially have trouble choosing a subset of crucial predictors, which would increase the variability of its estimates. In these situations, elastic net – which incorporates both $\lambda_1$ and $\lambda_2$ penalties – can offer greater stability. However, both lasso and elastic net may be prone to overfitting when the dataset is relatively small. Furthermore, the number of observations may have an impact on the selection of the ideal regularization parameters, which are established through cross-validation. The intricate interplay of bias, variance, and regularization effects in the connection between n and model performance calls for careful evaluation based on the particulars of the data and the goals of the modelling.

### 2.7.2. Changing the values of p

Changes in the number of predictors (p) have a considerable impact on lasso and elastic net performance. The difficulties in choosing significant predictors become increasingly apparent as the dataset's complexity rises, particularly for lasso. Lasso typically has trouble efficiently reducing the set of relevant features when there are more predictors than data, which could result in more varied coefficient estimates. Elastic net adds an extra regularization layer by combining $\lambda_1$ and $\lambda_2$ penalties,

which can improve stability in high-dimensional environments. But a significant increase in the number of predictors could also raise the possibility of overfitting, especially if the sample size is still small. In both cases, the dimensionality of the data may have an impact on the regularization parameter selection, which is critical. Therefore, in order to obtain optimal model performance, the influence of modifying the number of predictors should be carefully evaluated, combining the necessity of feature selection with the difficulties presented by high-dimensional data.

### 2.7.3. Changing the values of σ

We aim to explore the association between the parameter sigma (σ) and the penalties imposed by both the lasso and elastic net methods. This parameter introduces a degree of randomness and volatility to our simulated dataset Y. As the value of σ increases, the level of unpredictability and randomness in our Y also intensifies. We find that the elastic penalties with $\hat{\lambda}_2 = 0$ converge toward the lasso penalties when we decrease the variance in our simulation. Under such circumstances, the elastic net does not yield outcomes that are superior than the lasso problem. On the other hand, the mean mean-squared error of the elastic net performs better than the MSE of the lasso when we reverse this tendency and raise the randomization value σ. This is especially true in cases where $\hat{\lambda}_2$ is statistically larger than zero. Furthermore, there is a negative association between the number of estimated non-zero predictors and the parameter σ. A decrease in the count to correspond with the actual number of variables indicates that a higher σ results in better variable selection.

## 2.8. Conclusion

We can summarise our findings and results as follows.

### 2.8.1. Summary

We first developed the 'one-at-a-time' coordinate descent type of algorithm to solve the penalized regression problems – the lasso problem and elastic net. Our aim was to analyse the predictive accuracy of each and to also see which performed better at variable selection.

We simulated datasets, using the default parameter values as:

- n = 240
- $\beta$ = (3, 1.5, 0, 0, 2, 0, 0, 0)'
- $\sigma$ = 3
- The pairwise correlations between $X_i$, $X_j$ is determined as: $corr(X_i, X_j) = 0.5^{|i-j|}$
- r (number of simulations of the entire process) = 50

To select the optimal tuning parameter we ran the algorithm using trial values in the range of 0 to 5 with an increment of 0.1. Subsequently, the model is re-estimated on the training data using the optimal tuning parameters, and final results are obtained by evaluating it on the test data.

### 2.8.2. Results

We obtain results for various cases and settings.

**In the case n > p**:

Within a loop iterating over 50 simulations, datasets are generated with uncorrelated predictors, and cross-validation is employed to estimate optimal regularization parameters. The data is then split into training and test sets, and lasso and elastic net models are fitted using coordinate descent algorithms.

From our numerical results we note that:

- The mean of MSE for lasso is greater than the mean of MSE for elastic net. The standard error of MSE for lasso is greater than standard error of MSE for elastic net. Thus, we can conclude that **the elastic net has a better predictive performance** than lasso.
- On average the number of estimated non-zero coefficients selected by lasso is less than that for elastic net. Hence, we can conclude that **the elastic net regularization does better than the lasso at variable selection**.

**In the case p > n**:

When p is significantly larger than n, the elastic net penalty demonstrates greater efficiency compared to lasso, especially when data availability is limited for estimating numerous coefficients. Conversely, when the number of variables is small, the elastic net regularization tends to converge towards lasso regularization.

# Appendices

## References


- Friedman, J., Hastic. and Hofling, H. (2007). Pathwise coordinate optimization, The Annals of Applied Statistics 1: 302 - 332.
- Tibshirani, R. (1996). Regression shrinkage and selection via the lasso, Journal of Royal Statistical Society, Series B 58: 267 - 288.
- Tseng, P.(1988). Coordinate ascent for maximizing nondifferentiable concave functions, Technical Report.
- Tibshirani, R. (2001) Convergence of block coordinate descent method for nondifferentiable maxi- mization, J.Opt. Theory Appl. 109: 474 - 494.
- Iyer, S., Kitson, M. and Toh, B., 2005. Social capital, economic growth and regional development. Regional studies, 39(8), pp.1015-1040.